micress®

User Guide Version 6.2

Volume 0: MICRESS Phenomenology

"Resolution of partial differential equations is more about art than science".

Apocryphal quotation from Numerical Recipes in Fortran

"2 + 2 = 4 except for large values of 2"

Anonymous

"42"

Douglas Adams

This volume has been edited by:

MICRESS group

Contents

1 Introduction 4

2 An engineering approach to microstructure modeling 6

3 Basic model development 11

3.1 Aspects of multiphase equilibria 11
3.2 Sharp interface asymptotics 12
3.3 Aspects of computational efficiency 12
3.4 Coarsening and grain growth phenomena 12
3.5 Coupling to concentration fields including solute diffusion 12
3.6 Considering fluid flow 13
3.7 Coupling to thermodynamic databases 13
3.8 Incorporation of nucleation phenomena 13
3.9 Incorporation of elasticity/plasticity 14
3.10 Self-consistent coupling to macroscopic simulations 14

4 Applications to technical alloy grades 15

4.1 Steels 15
4.1.1 Solidification of steels 15
4.1.2 Gamma-alpha transition 15
4.1.3 Pearlite formation 16
4.1.4 Grain growth 16
4.2 Cast iron 16
4.3 Superalloys 17
4.4 Al alloys 17
4.5 Mg-Alloys 18
4.6 Solders 18
4.7 Intermetallic compounds 19
4.8 Other alloy systems 19

5 Present developments 20

5.1 Integrative Computational Materials Engineering 20
5.2 Determination of effective properties from simulated microstructures 20

6 Future directions 22

6.1 Data generation by numerical methods 22

7 References 23

1 Introduction

Any production is based on materials becoming components of a final product. Materials properties thus are of great importance for productivity and reliability of processing during production as well as for application and reliability of product components. A sound prediction of materials properties therefore is highly important. Material properties are highly linked to their internal microstructure and properties evolution along the entire component life-cycle, starting from a homogeneous, isotropic and stress-free melt and eventually ending in failure under operational load, is accompanied by microstructure formation and further evolution.

Scope of this handbook is to review the current state of the art with respect to simulation of microstructure evolution based on the phase-field approach in technical alloy grades. Starting from a short overview about computational thermodynamics and kinetics and respective databases for technical alloys, an engineering approach to phase-field and multiphase-field models will be depicted in order to allow for a basic explanation of these methods – in general being developed by physicists and mathematicians - for materials scientists and metallurgists.

Binary and ternary phase diagrams being available in printed form in books or publications have provided the basis for the development of materials ever since. Increasing availability of computers has allowed for the continuous development of computational thermodynamics and respective databases in the last decades.

Such software tools and databases are nowadays available for complex alloy systems comprising a number of alloy elements, e.g. [Thermo-Calc, Pandat, FactSage, JMatPro]. Their databases are established using a well-defined assessment scheme [Calphad]. They allow determining phase diagrams, calculating the sequence of phase transitions, the amount of phase fractions being stable at a given temperature and other thermodynamic properties, fig.1. Even more important for describing the evolution of a microstructure is that such models also allow the calculation of the driving forces for the phase transformations.

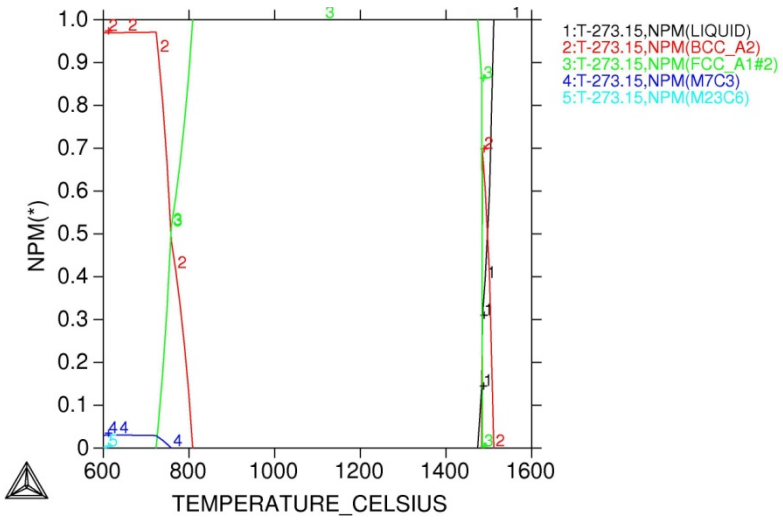

Figure 1.1 Equilibrium phase fractions of different phases in a 25MoCr4 steel as a function of temperature (calculated using Thermo-Calc and the TCFe6 database)

Continuing from the knowledge about equilibrium phase fractions - which do not provide any information about how fast this equilibrium is reached - subsequent developments aimed at describing the kinetics of diffusion controlled phase transitions. One example for a software tool especially suitable for the description of multicomponent diffusion using respective databases is [DICTRA]. The underlying approach here is based on 1-D systems like e.g. diffusion couples, concentric cylinders or concentric spheres. Under some specific assumptions phenomena like coarsening of a precipitate distribution can also be tackled.

Most interesting for metallurgists and materials engineers, however, is the microstructure and – even further– the properties of a material being based on its microstructure. The simulation of microstructures in technical alloy systems probably has its origin in the first dendrites being simulated using the phase-field method [Kobayashi 1993] and the subsequent extension of the phase-field method to multiple phase-fields [Steinbach 1996] allowing early simulations of eutectic and peritectic systems. This multiphase-field model later has been coupled to thermodynamic and mobility databases, thus providing the basis for all the examples on simulations of technical alloy grades being depicted in this paper. For reviews of these developments the reader is referred to [Steinbach 2007a], [Kitashima 2008], [Fries 2009] and [Steinbach 2009a].

2 An engineering approach to microstructure modeling

The phase-field method can be rigorously derived from thermodynamic principles and theories of phase transitions, and a lot of dedicated literature is available covering these fundamental and mathematical aspects (for a review see e.g. [Emmerich 2008],[Hecht 2010]). In this paper we will give a phenomenological approach for a rather intuitive interpretation of the phase-field concept and equations.

The first step towards the simulation of the dynamics of microstructure evolution is the basic description of a static microstructure, fig 2.1. A simple approach is to use a so called order parameter ϕ for simulations of microstructure evolution in a simple solid/liquid system. ϕ itself is a function of space x and time t i.e. and may take values between 0 and 1. Metallurgists may relate $\phi = \phi(\vec{x},t)$ this order parameter to the fraction of a specific phase (e.g. ϕ corresponds to the fraction solid in fig. 2) to be present at a specific point of space x and at a specific time t.

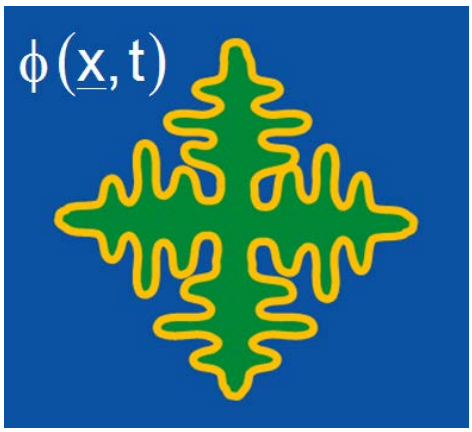

Figure 2.1 Description of a solidifying microstructure by an order parameter at a given moment t. The color coding is explained in the following:

$\phi(\vec{x},t)$ equals 1 :	100 % solid	0 % liquid
$\phi(\vec{x},t)$ equals 0 :	0 % solid	100 % liquid
$\phi(\vec{x},t)$ between 0 and 1 :	diffuse boundary	

This method of describing microstructures has been extended to the description of multiple grains and multiple phases in the multiphase-field method, where multiple, i.e. "i" different phase fields $\phi_i(\vec{x},t)$ denote the individual phases or even all different grains. In short, any object which can be identified in the microstructure may have its own phase-field variable in respective multiphase-field models.

Before entering multiphase-field models it seems wise to understand or at least to get a feeling for a description of the evolution of the simple solidification situation depicted in fig. 2.1. Describing the evolution of the microstructure thus means to identify the time derivative of the $\phi(\vec{x},t)$ i.e. the $\dot{\phi}(\vec{x},t)$.

A possible first step towards identification of a description of $\dot{\phi}(\vec{x},t)$ is to start from a diffusion equation (fig.2.2, blue contribution). A pure diffusion approach however would lead to a smear out of an initially sharp interface eventually ending up with a smooth and flat curve. In order to describe a stable, stationary interface an additional term thus is needed (fig. 2.2, green contribution), which stabilizes the interface. Note that this

contribution is negative for 0 < ϕ < 0,5 and positive for 0,5 < ϕ < 1. This term thus balances the effect of the diffusion term (blue) leading to a stationary, stabilized interface profile. Depending on the actual choice of this term, different stationary interface profiles may result (e.g. a hyperbolic tangent profile for a double well potential or a sine–profile for a double obstacle potential). Eventually any deviation from equilibrium (fig. 2.2, red contribution) will lead to a movement of the stationary interface profile. The deviation from equilibrium is characterized by ΔG. Depending on the sign of ΔG the motion will result either in growth or shrinkage of the respective phase. When equilibrium is reached (ΔG=0) the profile characterizing the interface position will become stationary and stable. Further variables in the respective equation denote the interfacial energy (σ), the interfacial thickness (η) and the interfacial mobility (μ):

$$\dot{\phi}(\vec{x},t) = \mu\left[\sigma\left(\nabla^2\phi - \frac{(1-\phi)(1-2\phi)\phi}{\eta^2}\right) + \frac{1}{\eta}\Delta G\,\phi(1-\phi)\right]$$

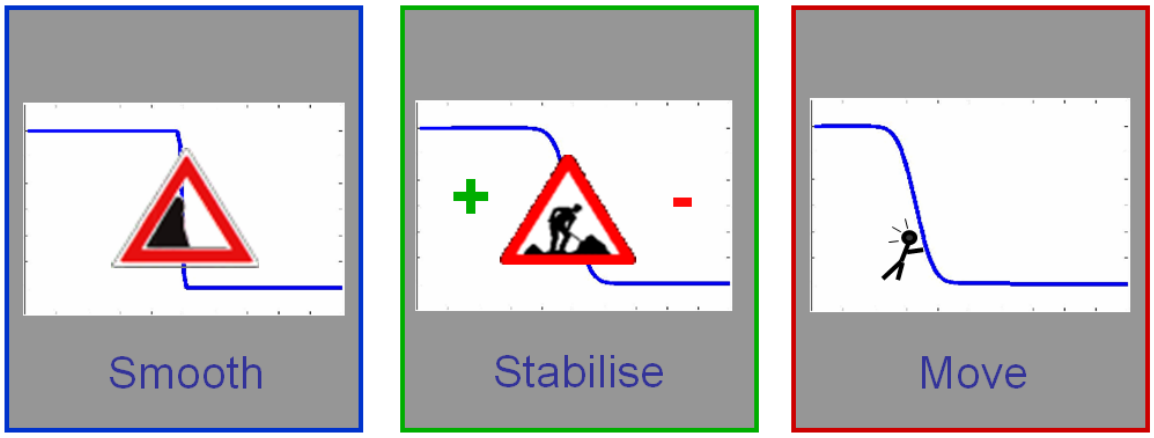

Figure 2.2 The phase-field equation in a very simple analysis. See text for explanation of the individual colors and terms of the equation (graphics: courtesy Nils Warnken, University of Birmingham)

Another engineering approach to the phase-field equation is based on the “Gibbs Thomson equation” giving a relation between interface velocity, thermal and solutal undercooling and interface curvature and being well known to metallurgists since decades [Diepers 1997], [Beckermann 1999].

A closer look at the phase-field equation (equation in fig. 2.2) reveals a rotational symmetry as the diffusion equation (fig 2.2, blue contribution) does not comprise any anisotropy. In order to include anisotropy into the model, both the interfacial energy σ and the interface mobility μ are assumed to be anisotropic. In 2 dimensions this can be accomplished by making these parameters dependant on the angle θ between the growth direction and the crystal orientation i.e. $\sigma = \sigma(\theta)$ and $\mu = \mu(\theta)$. For a simple cubic symmetry in 2D these functions could look like $\sigma = \sigma_0(1-\cos(4\theta))$ and $\mu = \mu_0(1-\cos(4\theta))$. For a hexagonal symmetry in 2 D functions like $\sigma = \sigma_0(1-\cos(6\theta))$ and $\mu = \mu_0(1-\cos(6\theta))$ would represent a first approach.

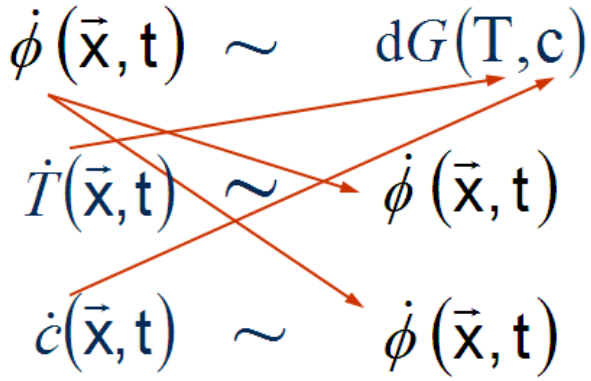

Figure 2.3 Evolving phase fractions influence e.g. the temperature field T by the release of latent heat or the concentration fields c_i due to the segregation of solute. These changes in turn alter the local conditions for the driving force dG.

Please note that in case of spatially varying interfacial energies the Gibbs-Thomson coefficient Γ has to be modified by including the second derivative of the interfacial energy:

$$\Gamma = \frac{\sigma}{L_0 T_m} \qquad \text{turns into} \qquad \Gamma = \frac{\sigma - \sigma''}{L_0 T_m}$$

In order to describe anisotropy in 3D configurations a more complicated description becomes necessary. A possible approach is the use of linear combinations of spherical harmonics [Eiken 2010b,c]. This approach allowed for description of the three dimensional growth of dendrites in Mg-alloys, fig.4.4

The driving force ΔG depends on local conditions of external fields like temperature T or concentration ci of the i different alloy elements (but also: stresses/strains, electric/magnetic fields, ...): $\Delta G = \Delta G(T,ci,..)$. A non-vanishing ΔG will lead to a finite change in phase fraction i.e. a finite $\dot{\phi}(\vec{x},t)$. This change in phase fraction in turn will affect the external fields, fig. 2.3. Thus there is a need of solving the coupled system of partial differential equations for the phase-field (in multiphase-field models: the multiple phase fields) and for all external fields affecting the phase transition.

Technical alloys comprise multiple grains, multiple phases and multiple components. Their description in numerical models requires at least the introduction of multiple phase fields, the description of multicomponent diffusion and thermodynamic and kinetic data. The basic ideas of the multiphase-field approach [Steinbach 1996] are:

- Definition of one phase field for each phase and for each grain of a phase
- Pairwise interaction for each pair of phases/grains like in standard phase-field
- Possibility of implementation of specific phase boundary/grain boundary properties

Further conceptual aspects comprise coupling to concentration fields [Tiaden 1999a] use of thermodynamic databases resp. mobility databases, multiphase interactions and physics of triple junctions

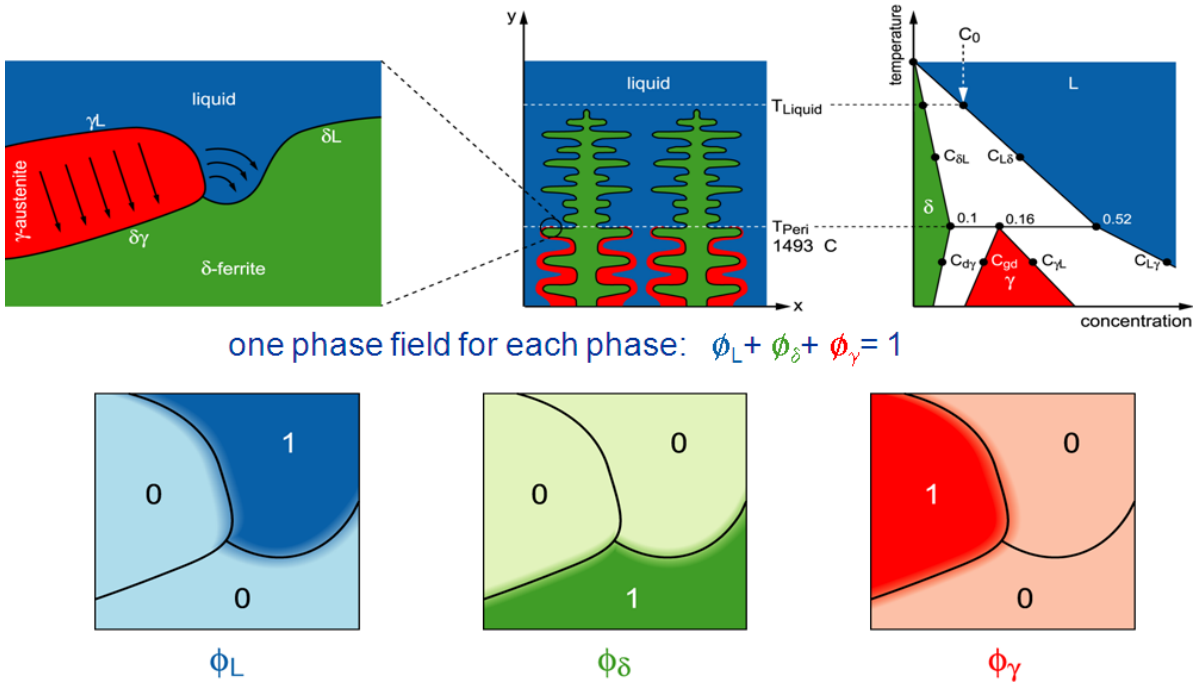

Figure 2.4 Schematic example of the multiphase-field approach for the peritectic solidification of steel. One order parameter is assigned to each of the phases liquid (L), δ and γ. The multiphase-field approach thus allows for the description of multiphase equilibria at triple junctions like eutectics or peritectics which occur in general when solidifying technical alloy systems. The concept is also applicable to solid state transformations like eutectoid transformations

The evolution of an initial state comprising multiple phases into a final state (denoted by prime) comprising the same phases can be realized as a rotation matrix operating onto the initial state while keeping its norm (i.e. the sum of all phase fractions) constant at a value of 1:

$$\begin{bmatrix} \phi_l \\ \phi_\delta \\ \phi_\gamma \end{bmatrix}' = \begin{bmatrix} \phi_{ll} & \phi_{l\delta} & \phi_{l\gamma} \\ \phi_{\delta l} & \phi_{\delta\delta} & \phi_{\delta\gamma} \\ \phi_{\gamma l} & \phi_{\gamma\delta} & \phi_{\gamma\gamma} \end{bmatrix} \begin{bmatrix} \phi_l \\ \phi_\delta \\ \phi_\gamma \end{bmatrix}$$

This matrix may be split into an identical matrix with 1 on the diagonal and an antisymmetric matrix comprising "transitions" between the individual phase-pairs:

$$\begin{bmatrix} \phi_l \\ \phi_\delta \\ \phi_\gamma \end{bmatrix}' = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \phi_l \\ \phi_\delta \\ \phi_\gamma \end{bmatrix} + \begin{bmatrix} 0 & \phi_{l\delta} & \phi_{l\gamma} \\ -\phi_{l\delta} & 0 & \phi_{\delta\gamma} \\ -\phi_{l\gamma} & -\phi_{\delta\gamma} & 0 \end{bmatrix} \begin{bmatrix} \phi_l \\ \phi_\delta \\ \phi_\gamma \end{bmatrix} \qquad \begin{bmatrix} \phi_l' - \phi_l \\ \phi_\delta' - \phi_\delta \\ \phi_\gamma' - \phi_\gamma \end{bmatrix} = \begin{bmatrix} 0 & \phi_{l\delta} & \phi_{l\gamma} \\ -\phi_{l\delta} & 0 & \phi_{\delta\gamma} \\ -\phi_{l\gamma} & -\phi_{\delta\gamma} & 0 \end{bmatrix} \begin{bmatrix} \phi_l \\ \phi_\delta \\ \phi_\gamma \end{bmatrix}$$

Such an interpretation has been one of the ingredients for the early development of the multiphase-field method, the transition matrix elements then being related to the "binary" transitions known from the classical phase-field equation e.g. for the solid/liquid system. Please note that these matrix elements have to be considered as operators and not as a pure multiplication and further simplifications have been made here to demonstrate the basic idea.

A detailed derivation is given in [Steinbach 1996]. For the solid/liquid system the order parameter ϕ has been identified as the fraction of the solid phase $\phi(\vec{x}) = \phi_S(\vec{x})$ and for the binary solid/liquid system the fraction of the liquid phase thus is given as $\phi_l(\vec{x}) = 1 - \phi_S(\vec{x})$. Rewriting the equation in figure 2.2 in terms of $\phi_l(\vec{x})$ and $\phi_S(\vec{x})$ then yields:

$$\dot{\phi}_S = \mu_{Sl}\left[\sigma_{Sl}\left(\nabla^2\phi_S - \frac{\phi_S\phi_l}{\eta_{Sl}^2}(\phi_S - \phi_l)\right) + \Delta G_{Sl}\frac{1}{\eta_{Sl}}\phi_S\phi_l\right]$$

The interface mobilities, interface energies, interface width and the driving force have been complemented by indices "sl" indicating their relation to this particular transition. This formulation allows assigning different properties like e.g. interfacial energies for each of the individual phase interactions in multi-phase systems. For the ternary situation depicted in fig. 2.4, the evolution of the liquid phase fraction would e.g. be described as a sum over the interactions with the δ-ferrite and the γ-austenite:

$$\dot{\phi}_l = \mu_{\delta l}\left[\sigma_{\delta l}\left(\nabla^2\phi_l - \frac{\phi_\delta\phi_l}{\eta_{\delta l}^2}(\phi_\delta - \phi_l)\right) + \Delta G_{\delta l}\frac{1}{\eta_{\delta l}}\phi_\delta\phi_l\right] + \mu_{\gamma l}\left[\sigma_{\gamma l}\left(\nabla^2\phi_l - \frac{\phi_\gamma\phi_l}{\eta_{\gamma l}^2}(\phi_\gamma - \phi_l)\right) + \Delta G_{\gamma l}\frac{1}{\eta_{\gamma l}}\phi_\gamma\phi_l\right]$$
$$+ \textit{higher order junction terms } J_{l\delta\gamma}$$

3 Basic model development

Starting from the initial idea of describing microstructure evolution in multiphase systems [Steinbach 1996] a number of further developments was necessary to make the model applicable and useful for technical alloy systems. The respective major topics are shortly outlined in the following and the reader is referred to respective articles for further reading.

In detail – amongst others - the following topics have continuously been addressed since 1996:

- aspects of multiphase equilibria
- sharp interface asymptotics
- aspects of computational efficiency
- coarsening phenomena
- coupling to concentration fields including solute diffusion
- consideration of fluid flow
- coupling to thermodynamic databases
- incorporation of nucleation phenomena
- incorporation of elasticity/plasticity
- self-consistent coupling to macroscopic simulations

3.1 Aspects of multiphase equilibria

One of the major questions arising shortly after publication of the first model was, whether the multibinary description of a triple junction was sufficient to describe the correct equilibrium situation being macroscopically defined by Young's law or whether additional terms have to be introduced into the formulations. The need for such additional terms is identified in a number of publications [Nestler 1998],[Nestler 2002]. From an engineering perspective such terms may also be related to catalyst reactions, where the mere presence of a third phase influences the transition between two other phases.

3.2 Sharp interface asymptotics

Solution of the system of partial differential equations (PDEs) on a reasonable grid size leads to an unphysical interface thickness of some numerical grid cells (in contrast to the physical thickness of some monolayers). Nevertheless, the paradigm behind phase-field modelling is that the phase-field method is able to reproduce the sharp interface solutions, e.g. the Gibbs-Thomson equation in a solidification problem. From the numerical point of view, this asymptotic is not feasible because this would require a numerical interface thickness on the scale of the physical interface thickness. [Karma 2001] , however, could show how corrections for artefacts evoked by this artificial numerical interface thickness become possible in the framework of "thin interface asymptotics", where the limiting length scale is the diffusion length l_d, i.e. in cases where $l_d > \eta$. These corrections speed up simulations tremendously. Further important work towards quantitative phase-field modeling has been contributed by Plapp and co-workers [Plapp 2002],[Folch 2005],[Echebarria 2004].

3.3 Aspects of computational efficiency

The numerical solution of the coupled system of a large number of partial differential equations requires a high computational efficiency. In contrast, the correct resolution of details of the microstructure requires a very fine meshing. Besides solving the coupled system of PDE's only at the interfaces using interface fields [Steinbach 1999a] especially adaptive grids providing a local remeshing at the interfaces have turned out to be beneficial [Provatas 1998],[Provatas 1999],[Ofori 2010]. In view of coupling with thermodynamic databases, a multibinary extrapolation scheme reduces the computational load as compared to regular calls to databases [Eiken 2006].

3.4 Coarsening and grain growth phenomena

Even in absence of any explicit thermodynamic driving force, the phase-field equations lead to a further evolution of the microstructure as the respective equations tend to minimize the total interfacial area of the system as is also noted in the Allen-Cahn equation [Allen 1979], which represents one of the roots of the phase-field method. Available work on coarsening phenomena comprises Ostwald ripening of solids in a liquid alloy with or without fluid flow [Diepers 1999] or grain growth in solids [Fan 1997] [Moelans 2006] [Moelans 2008] with or without stresses in pure substances and in alloys. Respective investigations have also addressed ideal grain growth [Schaffnit 2007] and later have been extended to phase-field models comprising pinning of grain boundaries by impurities, a recent overview is [Apel 2009a].

3.5 Coupling to concentration fields including solute diffusion

Coupling to concentration fields was first discussed for isothermal phase transitions in binary alloys by [Wheeler 1992]. One of the challenges to allow for the description of technical alloys was the correct treatment of solute redistribution and the calculation of the driving forces across diffuse interfaces revealing a numerically finite thickness. This has been first realized for a multiphase binary system [Tiaden 1998], [Kim 2004]. Aspects of combined heat and solute diffusion during solidification of a binary alloy have been treated by [Ramirez 2004].

While diffusion in binary alloys can still be handled by a single diffusion equation, the simulation of diffusion in complex alloy system is much more challenging in view of effects like cross-diffusion (e.g. uphill diffusion of one alloy element in the gradient of another alloy element). For simulation of complex alloy systems the consideration of the full diffusion matrix can be mandatory. Regarding the amount of diffusion data necessary

for a technical alloy system, the use of available mobility databases thus is very attractive. This can be achieved via online-coupling to thermodynamic and mobility databases [Böttger 2000], [Eiken 2006].

3.6 Considering fluid flow

Besides diffusion, fluid flow is a major transport mechanism for species and heat. In general fluid flow however takes place on a larger length scale as compared to the evolution of the microstructure and thus may be considered by selecting suitable boundary conditions for a microstructure simulation. But also on the scale of the microstructure itself fluid-flow has significant influence on coarsening [Diepers 1999], dendrite growth morphology [Beckerman 1999], [Steinbach 2009b], and on dendrite spacing selection [Diepers 2002a], [Diepers 2002b], [Diepers 2006], [Zimmermann 2009]. When implementing fluid flow into phase-field models, the well known “no-slip”-boundary condition for flow at interfaces has to be modified in order to account for the finite thickness of the diffuse interface. This has been realized by introduction of an interfacial stress term varying across the thickness of the diffuse interface [Beckermann 1999].

3.7 Coupling to thermodynamic databases

Crucial for modelling of multicomponent and multiphase technical alloys is a proper description of the thermodynamic properties of the alloy. The CALPHAD approach [Calphad] has proven to be very powerful for calculating phase equilibria in complex alloy systems. Databases for many important classes of technical alloys are available nowadays, e.g. [Thermo-Calc, JMatPro, FactSage, Pandat], putting together a vast quantity of experimental data in binary, ternary and higher order alloy systems. Mobility data for some alloy systems are available as well [Thermo-Calc].

A consequent continuation of this idea is the online coupling of such databases to the multiphase-field model by replacing the global equilibrium consideration with local equilibrium conditions. The first steps in this direction have been made by coupling e.g. the thermodynamic software Thermo-Calc [Thermo-Calc] to a multiphase-field model [Steinbach 1996], using the TQ Fortran interface [Grafe 2000 a,b,c], [Böttger 2000]. From these early models, the quasi-equilibrium approach was developed [Eiken 2006], which is implemented in the software package MICRESS® [MICRESS] and has been successfully applied to different alloy systems as described below. Comprehensive reviews about coupling of thermodynamic data to phase-field models detail a number of different aspects: [Qin 2005], [Steinbach 2007a], [Kitashima 2008], [Fries 2009] and [Steinbach 2009a].

3.8 Incorporation of nucleation phenomena

Nucleation typically takes place on a much smaller length scale than the further evolution of microstructure. In spite of the fact, that nucleation can in principle be described by phase-field models on that small length scale [Granasy 1994], [Warren 2009], the description of nucleation in simulations on the scale of individual grains has to draw back on other nucleation models. A variety of models have been implemented to phase-field codes allowing e.g. to assign different nucleation probabilities in the bulk volume of the phases as compared to nucleation at interfaces and triple or higher order junctions. Seed density models have been integrated to allow for different numbers of nuclei to become active dependant on the local undercooling [Böttger 2006a] [Böttger 2009a].

3.9 Incorporation of elasticity/plasticity

Solid state transformations are often accompanied by elastic deformation or even plastic deformations. Both phenomena can be naturally integrated into the phase-field concept, because both contribute to the driving force for the phase transformation although a thermodynamic interpretation of plasticity is still subject of ongoing discussions. Important contributions to the field of elasticity and phase-field have been made by [Katchaturyan 1999] and [Wang 2010]. Elasticity has been incorporated into the multiphase-field model [Steinbach 2006] and has been applied e.g. to describe the pearlitic transformation in steels [Steinbach 2007c]. Nowadays it can be also used to derive effective mechanical engineering constants e.g. the Young's modulus from simulated, complex multiphase microstructures [Laschet 2010]. Effects of inelastic deformations on solid state transformations have been investigated in [Benke 2008].

3.10 Self-consistent coupling to macroscopic simulations

Consistent coupling of microstructure simulation to macroscopic temperature fields in technical processes like e.g. sand castings is not an easy task, because latent heat plays an important role: While latent heat production is directly linked to microstructure formation, heat conduction is rather a phenomenon on the macroscopic length scale. Thus, a temperature solution which is consistent with microstructure formation can only be obtained directly, if microstructure is solved simultaneously on the whole casting. This, obviously, is impossible if complex and time-consuming microstructure models like the phase-field method are used.

Recently, an iterative approach was developed to achieve self-consistency between the macroscopic temperature evolution and microstructure formation, which has been applied to an equiaxed AlCu casting [Böttger2009a],[Böttger2009b]. The approach couples a one-dimensional macroscopic temperature field to a multiphase-field model using the homoenthalpic approximation, which assumes a unique enthalpy-temperature curve across the casting. It has been shown that consistent coupling between the micro- and macro-scale was important for a correct microstructure prediction, and that consistency was achieved after very few iterations.

4 Applications to technical alloy grades

The following chapters will describe investigations and developments aiming at the description of microstructure evolution in technical alloy grades, which have been performed with the help of the software MICRESS® [MICRESS]. They will address steels, cast iron, superalloys, Al- and Mg-alloys, solders, intermetallic compounds and other alloys/systems. Along with the evolution of the underlying model basis, the phenomena being tackled have become increasingly sophisticated for each of these materials.

4.1 Steels

Already in ancient times the complex interplay between diffusion, precipitation, dissolution and re-precipitation as well as their control by well defined process scenarios has been exploited to develop sophisticated steel grades, like e.g. the damascene steel revealing high-tech structures on the micro and even nano-scale. It is however worth noting that approximately 70% of the present 2500 different steel grades have been developed during the last twenty years. Steels provide a variety of different phenomena occurring both during solidification and during subsequent solid state transformations, the microstructure resulting from the preceding process step in most cases being of major importance for its further evolution during the subsequent steps. Probably for this reason, steels have been the first technological materials being investigated by multiphase-field methods.

4.1.1 Solidification of steels

First activities aimed at modeling the peritectic solidification in a binary Fe-C system [Tiaden 1999]. Recent work describes modeling of the solidification of technical steel grades [Böttger 2008b], [Fukumoto 2009] and also addresses aspects like hot ductility during solidification of steel grades in continuous casting processes [Böttger 2010], [Senk2010].

The phenomena considered in such simulations comprise e.g. the formation of MnS precipitates, effects of cross-diffusion leading to inverse segregation of specific elements like P, the formation of segregation bands as consequence of discontinuous solidification conditions and many others.

4.1.2 Gamma-alpha transition

Next step for the microstructure evolution in technical steel grades are solid state transformations, especially the gamma-alpha transition. This phenomenon has first been modelled in 2D in 2001 [Pariser 2001], [Pariser 2006] and be further extended and experimentally verified [Mecozzi 2003], [Mecozzi 2005], [Mecozzi 2007] and applied to model the heat affected zone during welding of low carbon steel [Thiessen 2006 a,b,c]

Recent simulations of the gamma-alpha transition in 3D reveal the importance of different nucleation sites not occurring in 2D simulations like quadruple points or triple lines [Militzer 2006] and the effects of stresses affecting the transition [Apel 2009b].

Work on austenitization upon heating indicates this process not being the simple reverse of the ferrite formation [Savran 2009]. Nucleation of austenite may start from ultrafine ferrite-carbide aggregates [Azizi 2010]. The successful use of a recently developed NPLE (non-partitioning, local equilibrium) model was demonstrated by simulation of austenite formation from an experimental ferrite plus pearlite microstructure and comparison to experimental results [Rudnizki 2010d].

4.1.3 Pearlite formation

Pearlite transformation is a well-known eutectoid transformation, where a solid parent phase decomposes into two solid phases simultaneously. It is similar to eutectic solidification, where the phase state of the parent phase is the liquid. Both transformations can lead to a lamellar microstructure, and diffusion plays a major role for the spacing selection in this structure.

First multiphase-field investigations on pearlite formation thus addressed the diffusion in both ferrite and austenite and aimed at describing the resulting spacing/growth rate. Respective results [Nakajima 2006] already predicted a larger growth rate as compared to classical theoretical models [Zener 1947], [Hillert 1957] but still could not close the discrepancies with experimental observations.

Further investigations revealed that the transformation strain inhibits the cooperative growth mode of cementite and ferrite and provokes the salient growth of cementite needles ahead of the ferrite front. The predicted growth velocities are in the right order of magnitude as compared to the experiment and thus close the gap between predictions by classical models being based on diffusion only and experimental observations [Steinbach 2007c].

While all above simulations locally resolve the distinct thermodynamic phases of the pearlite (i.e. ferrite and cementite), present model developments aim at describing pearlite as an “effective” phase without resolving the individual ferrite-cementite lamella [Thiessen 2007]. For this purpose a combination of thermodynamic descriptions taken from databases and of linearized “phase-diagrams” for the pearlite pseudo phase has recently been implemented into a multi-phase-field code [MICRESS].

4.1.4 Grain growth

Phase-field models do not always require an explicit thermodynamic driving force to drive the evolution of a microstructure. Because the respective equations can be derived from the Gibbs-Thomson relation, they implicitly tend to minimize curvature and thus allow for the description of ripening and grain growth. Subsequent to models for ideal grain growth [Schaffnit 2007], effects of particle pinning on the mobility of the grain boundaries have been included [Apel 2009a], fig 4.1. Respective models now allow for the description of abnormal grain growth [Rudnizki 2010a], e.g. during case hardening [Rudnizki 2010b,c] or for the description of grain growth in microalloyed line-pipe steels [Schaffnit 2009], [Schaffnit 2010], [Tolui 2010], [Fayek 2010].

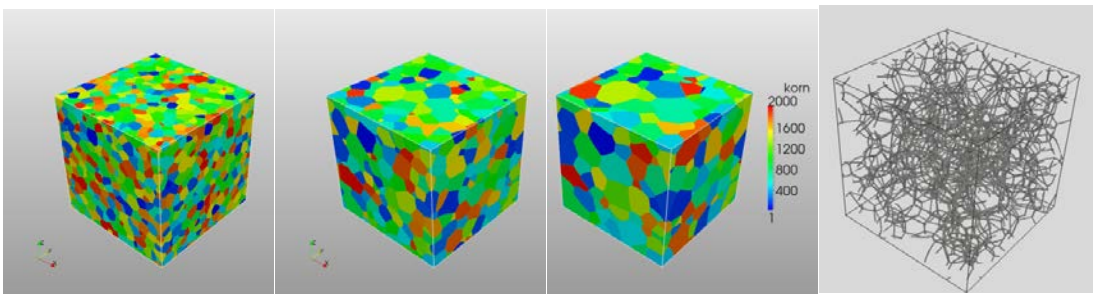

Figure 4.1 3D grain growth simulation for different time steps starting from 2000 individual grains. Color coded are the individual grains (left). On the right: representation of the triple lines of intersecting grain boundaries.

4.2 Cast iron

Few simulations in the area of cast iron have by now addressed aspects of nucleation conditions for graphite in dependence on the segregation profile of different alloy elements. In a simulation study [Sommerfeld 2008], nucleation of graphite on MnS particles, which form during solidification, has been identified as a possible scenario for formation of lamellar graphite in gray iron. Based on this scenario, especially the titanium composition turned out to be a decisive factor: Too high levels of titanium lead to suppression of nucleation and poor development of graphite lamellae. Respective simulations could be confirmed by experiments.

Figure 4.2 Solidification simulation in cast iron. The formation and the growth of tiny MnS particles in the liquid influence the subsequent formation of graphite [Sommerfeld 2008]

4.3 Superalloys

Nickel-based superalloys find widespread use in high-temperature applications, e.g. in turbines for aero-engines, gas or steam turbines for power generation [Rösler 2003][Herzog 2006]. Many of the respective components like turbine blades and/or vanes are produced using methods of investment casting and subsequent directional solidification. Solidification can then cause melt-related defects in these components. The morphological evolution of the dendritic structure and the subsequent solid-state transformations upon cooling and homogenization heat treatments thus are important for applications.

Multiphase-field models coupled to thermodynamic databases can account for the full compositional complexity of technically relevant superalloys [Warnken 2007]. Microsegregation, the phase fractions in the as-cast and directionally solidified [Ma 1999],[Grafe 2000c],[Böttger 2000] microstructures, formation of eutectic islands [Warnken 2005] the solidification-rate dependent dimensions of the mushy zone and the sequence of phase formation can be correctly predicted For phase transformations occurring during solidification effects of back-diffusion have been identified as being important. Extensions of the method which include homogenization of the as-cast microsegregation have been demonstrated [Warnken 2008] [Warnken 2009]. Recent studies have addressed the long term behavior (> 100.000 h) of precipitates in technical superalloy grades [Böttger 2010, unpublished].

4.4 Al alloys

In the field of aluminum alloys, there is a high interest in microstructure simulation originating from automotive industry being caused by demands for lightweight alloys with optimized mechanical properties. Consequently, several approaches for the simulation of microstructure formation in technical aluminum alloys have been used by now, incorporating thermodynamic data on different levels [Kovacevic 2008],[Qin 2005],[Wang 2009]. The multiphase-field model [Eiken 2006] with direct coupling to thermodynamic data bases has been used for the calculation of microsegregation in the hypoeutectic alloy AA6061, the widely used A356 casting alloy, and eventually the slightly hypereutectic piston alloy KS1295 comprising up to 14 thermodynamic phases [Böttger 2009c].

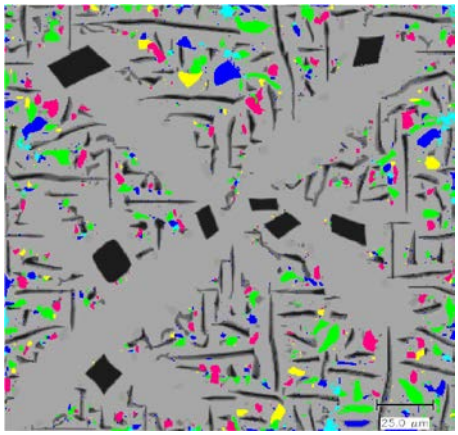

Figure 4.3 Simulation of the solidification of a commercial Al alloy grade comprising seven alloy elements. Some of these alloy elements tend to form intermetallic phases, and a total of 14 different thermodynamic phases has been considered in this simulation [Böttger 2009c].

Recent work on Al-Alloys comprises effects of flow on dendritic growth [Zimmermann 2009], simulations on grain refinement [Nomoto 2009], rheo-casting of Al alloys [Bünck 2010] and porosity formation during solidification of A356 [Carre 2010].

4.5 Mg-Alloys

Mg-based alloys are gaining increasing technical importance due to the high demand for weight reduction, especially in transportation industry. A specific feature of magnesium solidification is the hexagonal anisotropy of the hcp lattice.

Equiaxed solidification of the magnesium alloy AZ31 has been simulated using a two-dimensional hexagonal anisotropy and a seed density model for the description of nucleation of the primary dendrites [Böttger 2006b]. Major objectives of further studies were the influence of alloy composition and process parameters on the grain size [Eiken 2007], [Eiken 2010b,c]

Phase-field simulations of solidification of Mg-alloys in three dimensions have been applied in order to investigate the role of the Mg-specific hexagonal dendrite morphology in the process of competitive grain growth and the resulting selection mechanisms [Eiken 2009a], [Eiken 2010a,c]. Further work e.g. addresses the castability of technical Mg-alloy grades [Kahn 2009].

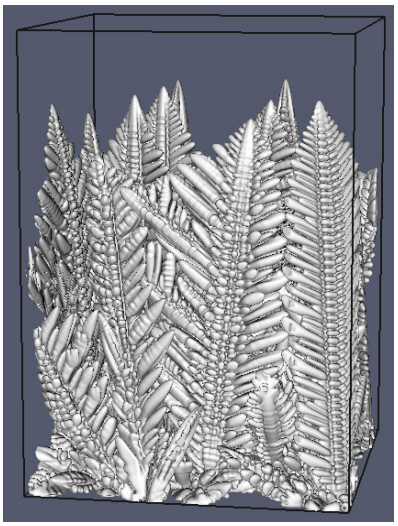

Figure 4.4 3D-simulation of texture evolution in Mg-6% Al. Only few grains prevail after a short distance of directional solidification. The simulation has been started from 50 initial nuclei being randomly oriented [Eiken 2010b,c].

4.6 Solders

Failure of electronic components often occurs at solder joints and particularly at microstructural features, like e.g. phase boundaries with intermetallics. Especially new solder alloys on the basis of ternary and higher alloyed

solder systems like Sn-Ag-Cu are gaining importance and cannot be easily described by analytical approaches. Increasing integration density moreover leads to additional constituent elements originating from either boards, components or from their surface finish. These constituents have also to be considered for microstructure evolution. In addition to recent thermodynamic and kinetic modeling describing the range of possible stable phases, the phase-field approach allows describing their spatial distribution. A respective microstructure [Schmitz 2009a] may serve as a basis for future lifetime and reliability prediction of the respective solder joint. Special interest may originate from modeling electric current distributions in the microstructure and their influence on inhomogeneous heating during operation of the joint or on electromigration of components affecting microstructure evolution.

4.7 Intermetallic compounds

The properties of modern TiAl-based intermetallic alloys critically depend on the solidified microstructure. Commonly, a rather coarse grain structure is obtained if α(Ti) forms via the peritectic reaction 'liquid + βTi) $\rightarrow\alpha$(Ti)'.

A multiphase-field model has been applied to qualitatively simulate the interaction between nucleation and growth of the peritectic α(Ti) in TiAl alloys with Al content varying between 43 and 47 at.% Al. With increasing aluminum content, the fraction of the pro-peritectic β(Ti) phase being present at the peritectic temperature decreases. A higher Al-content additionally increases the grain refining effect due to growth restriction [Eiken 2009b].

4.8 Other alloy systems

Besides applying multiphase-field models to structural material like those detailed above, there are also applications to functional materials like superconductors [Schmitz 1998], solar silicon [Apel 2002a,b],[Steinbach 2007b],[Steinbach 2000], coatings [De Bruycker 2004], Al-Zn-Si [Phelan 2004], rapidly solidified Ni-Zr-Al [Galenko 2009] , Cu-Al alloys [Kauzlaric 2008], and Nb-Si alloys [Amancherla 2007].

5 Present developments

5.1 Integrative Computational Materials Engineering

Recently, the high importance of an "Integrative Computational Materials Engineering" (ICME) for the future economic development and competitiveness has been strongly emphasized [NRC2008]. One of the major prerequisites for an efficient ICME is the definition of a common and open standard for information exchange between different simulation tools allowing daisy-chaining a number of different process simulation tools along the production chain and also coupling the different scales being relevant for microstructure evolution and accordingly for the resulting properties [Schmitz 2009b].

Results and boundary conditions from the macroscopic process simulations can be used as boundary conditions to model microscopic effects like abnormal grain growth during carburizing. The resulting microstructures for each step provide the basis for the determination of effective properties, which can be either used to optimize alloy concepts or can be coupled back as local values to the process simulations in order to improve their accuracy and predictive capabilities with respect to the final properties of the component.

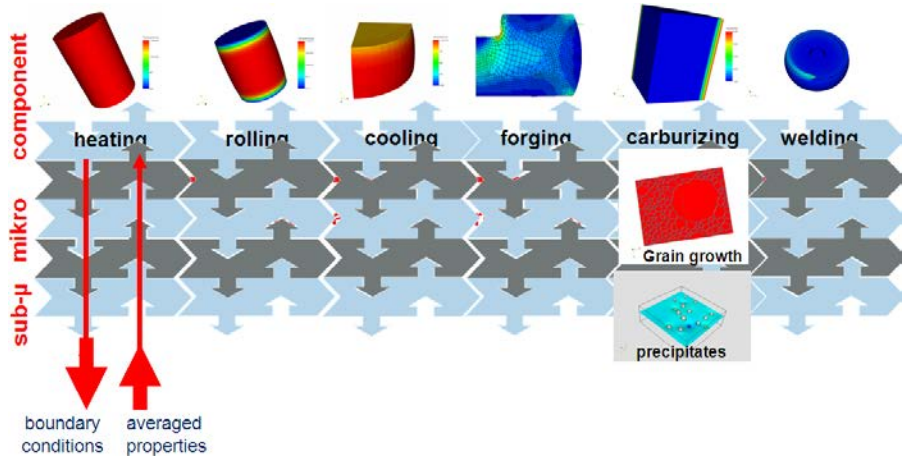

Figure 5.1 Sketch of a virtual platform for materials processing. The information exchange between different simulation tools on the component scale as well as the information exchange between different length scales is based on an open, standardized data format. This strategy allows tracking the influence e.g. of microsegregation during solidification on subsequent precipitate formation and eventually on grain stability during carburizing [Schmitz 2009b],[Rudnizki 2010a].

5.2 Determination of effective properties from simulated microstructures

Models of microstructure evolution provide a maximum information depth in the form of spatially and temporally resolved microstructures. To obtain information relevant for simulations on a larger length scale, a reduction of these data and an extraction of effective properties is mandatory. These effective properties are also most important for any alloy and process development and can be determined e.g. by methods of mathematical homogenization or by virtual testing.

The basic idea of mathematical homogenization is to calculate the effective properties of a composite structure like a multiphase microstructure of a real alloy on the basis of the knowledge of (i) the properties of the individual pure phases constituting the composite and (ii) their three dimensional topological arrangement.

Virtual tests are based on numerically mimicking experimental material tests like e.g. tensile tests with the adjusted boundary conditions from which the reproduced microstructure evolves.

Respective models by now have been applied to extract effective properties from microstructures simulated by the multiphase-field method from 2-phase and multi-phase structures in 3D [Apel 2009b] and to properties evolving during the gamma-alpha transition in steels. Another approach is the determination of effective properties from simulated microstructures by mathematical homogenization [Laschet 2010].

6 Future directions

6.1 Data generation by numerical methods

Although already quite an amount of data required to model microstructures is available in terms of thermodynamic databases and mobility databases, numerous parameters still have to be determined experimentally. Respective data comprise the temperature and composition dependant properties of the individual thermodynamic phases like thermal conductivities, bulk elastic moduli, density etc., but also the Gibb's energies for phases, where this value can experimentally only hardly be determined.

There is a perspective that respective data may be gained from ab-initio calculations and molecular dynamics simulations in the near future even for complex alloy systems. Even more interesting is the calculation of interfacial properties like interfacial energy and interfacial mobility including their anisotropies and their dependence on composition and temperature [Guerdane 2010].

In summary, phase-field and multiphase-field methods during the last decade have developed into powerful tools for materials engineering. The present situation may be compared to the development of FEM methods, which have revolutionized mechanical engineering about twenty years ago. Phase-Field methods are actually on the track to become the "FEM for metallurgists and materials scientists".

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